Ground state phases of the Half-Filled One-Dimensional Extended Hubbard Model

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Using quantum Monte Carlo simulations, results of a strong-coupling expansion, and Luttinger liquid theory, we determine quantitatively the ground state phase diagram of the one-dimensional extended Hubbard model with on-site and nearest-neighbor repulsions U and V. We show that spin frustration stabilizes a bond-ordered (dimerized) state for $U \approx V/2$ up to $U/t \approx 9$, where t is the nearest-neighbor hopping. The transition from the dimerized state to the staggered charge-density-wave state for large V/U is continuous for $U \lesssim 5.5$ and first-order for higher U.

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The one-dimensional Hubbard model, which describes electrons on a tight-binding chain with single-particle hopping matrix element t and on-site repulsion U, has a charge-excitation gap for any $U > 0$ at half-filling [1]. In the spin sector, the low-energy spectrum maps onto that of the $S = 1/2$ Heisenberg chain; the spin coupling $J = 4t^2/U$ for $U \to \infty$. The spin spectrum is therefore gapless and the spin-spin correlations decay with distance r as $(-1)^r/r$ [2]. Hence, the ground state is a quantum critical staggered spin-density-wave (SDW). In the simplest *extended Hubbard model*, a nearest-neighbor repulsion V is also included. The Hamiltonian is, in standard notation and with $t = 1$ hereafter,

$$\begin{aligned} H &= -t \sum_{\sigma=\uparrow,\downarrow} \sum_i (c^\dagger_{\sigma,i+1} c_{\sigma,i} + c^\dagger_{\sigma,i} c_{\sigma,i+1}) \\ &+ U \sum_i n_{\uparrow,i} n_{\downarrow,i} + V \sum_i n_i n_{i+1}. \end{aligned} \tag{1}$$

The low-energy properties for $V \lesssim U/2$ are similar to those at $V = 0$. For higher V the ground state is a staggered charge-density-wave (CDW), where both the charge and spin excitations are gapped. The transition between the critical SDW and the long-range-ordered CDW has been the subject of numerous studies [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. Until recently, it was believed that the SDW-CDW transition occurs for all $U > 0$ at $V \gtrsim U/2$ and that it is continuous for small U ($\lesssim 5$) and first-order for larger U. However, based on a study of excitation spectra of small chains, Nakamura argued that there is also a bond-order-wave (BOW) phase [10], where the ground state has a staggered modulation of the kinetic energy density (dimerization), in a narrow region between the SDW and CDW phases for U smaller than the value at which the transition changes to first order. Previous studies [6, 7, 8, 9] had indicated an SDW state in this region. Nakamura's BOW-CDW boundary coincides with the previously determined SDW-CDW boundary. The presence of dimerization and the accompanying spin gap were subsequently confirmed using quantum Monte Carlo (QMC) simulations [11, 12]. The BOW phase now also has a weak-coupling theory [13].

The existence of an extended BOW phase has recently been disputed. Jeckelmann argued, on the basis of density-matrix-renormalization-group (DMRG) calculations, that the BOW exists only on a short segment of the first-order part of the SDW-CDW boundary [14], i.e., that the transition always is SDW-CDW and that BOW order is only induced on part of the coexistence curve. However, QMC calculations demonstrate the existence of BOW order well away from the phase boundary [12].

Although several studies agree on the *existence* of an extended BOW phase [10, 11, 12, 13], the shape of this phase in the (U, V) plane has not yet been reliably determined. The system sizes used in the exact diagonalization study [10] were too small for converging the SDW-BOW boundary (i.e., the spin gap transition) for $U \gtrsim 4$. In the previous QMC studies [11, 12], the emphasis was on verifying the presence of BOW order and the phase transitions for $U \approx 4$. In this Letter, we present the complete phase diagram. Taking advantage of recent QMC algorithm developments—stochastic series expansion with directed-loop updates [15] in combination with the quantum generalization [11] of the parallel tempering method [16]—we have carried out high-precision, large-chain (up to $L = 1024$) calculations for sufficiently high U (≤ 12) to locate the point at which the BOW order vanishes. In agreement with Ref. [14], we find that the BOW exists also above the U at which the transition to the CDW state becomes first-order. However, long-range BOW order exists also below this point, and hence *the point at which the nature of the transition changes from continuous to first-order is on the BOW-CDW boundary.*

The phase diagram we find here is qualitatively similar to that obtained in a 4th order strong-coupling expansion, where the transition to the CDW state is de-

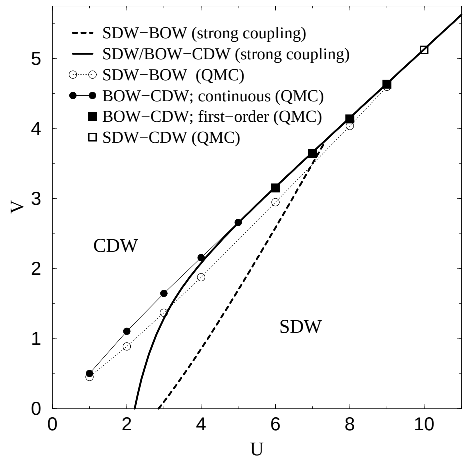

FIG. 1: QMC and strong-coupling phase diagram. The BOW is located between the SDW-BOW and BOW-CDW curves.

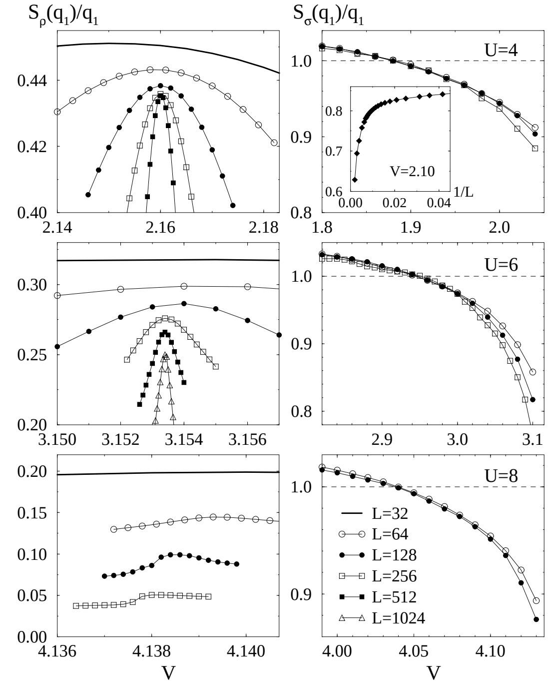

FIG. 2: Long-wavelength charge (left panels) and spin (right panels) structure factors vs V for $U = 4$ (top), 6 (middle), and 8 (bottom). The system sizes are indicated in the low-right panel. The $U = 4$ inset shows the dependence on the inverse lattice size at $V = 2.10$.

termined by comparing the energies of the large-V CDW state and the effective spin model including nearest- and next-nearest-neighbor interactions J and J' [8]. The BOW phase corresponds to the spontaneously dimerized phase of the spin chain, i.e., $J'/J > 0.241$ [17]. In Fig. 1, we compare our QMC phase boundaries with the strong-coupling result; the procedures giving the QMC boundaries will be discussed below. We will show that the system is a Luther-Emery liquid on the continuous BOW-CDW boundary, i.e., the charge gap vanishes and the spin gap remains open. Evidence supporting this type of transition was also presented in Ref. [11]. Here we will further argue that the change to a first-order transition corresponds to the Luttinger charge exponent K_ρ reaching the value $1/4$.

We extract the SDW-BOW and BOW-CDW boundaries using the charge and spin exponents K_ρ and K_σ. If there is a spin or charge gap, the corresponding exponent vanishes. Otherwise the equal-time correlation function $C_\rho(r) \sim r^{-(K_\sigma+K_\rho)}$, $C_\sigma(r) \sim r^{-(K_\sigma^{-1}+K_\rho)}$. If non-zero, the spin exponent $K_\sigma = 1$ as a consequence of spin-rotation invariance [18]. On periodic chains the exponents can be conveniently extracted from the static structure factors $S_{\rho,\sigma}(q)$ [19],

$$S_{\rho,\sigma}(q) = \frac{1}{L}\sum_{j,k} \mathrm{e}^{iq(j-k))}\langle(n_{\uparrow j} \pm n_{\downarrow j})(n_{\uparrow k} \pm n_{\downarrow k})\rangle, \quad (2)$$

in the limit $q \to 0^+$:

$$K_{\rho,\sigma} = S_{\rho,\sigma}(q_1)/q_1, \quad q_1 = 2\pi/L, \quad L \to \infty. \quad (3)$$

If there indeed are three successive phases, SDW-BOW-CDW, as V is increased at a fixed value of U, then the spin exponent $K_\sigma = 1$ in the SDW phase and $K_\sigma = 0$ everywhere else. The charge exponent $K_\rho = 0$ everywhere, except exactly at the BOW-CDW transition point if this is a continuous quantum phase transition (i.e., if the charge gap vanishes). In contrast, if the transition is first-order, then $K_\rho = 0$ also on the phase boundary. Using the relation (3) for a finite system, any discontinuities will naturally be smoothed, and one can only expect to observe $S_{\rho,\sigma}(q_1)/q_1$ developing sharp features as L is increased. In Fig. 2 we show results demonstrating this for several different system sizes at $U = 4$, 6, and 8.

Looking first at the charge exponent, if $K_\rho > 0$ on the BOW-CDW boundary and $K_\rho = 0$ elsewhere, then one can expect a peak developing in $S_\rho(q_1)/q_1$ versus V. The peak position corresponds to the critical V, and the peak height should converge to K_ρ. If the transition is first-order, $S_\rho(q_1)/q_1$ should converge to zero for all V, but one can still expect some structure at the phase boundary for finite L as the nature of the ground state changes. In Fig. 2, for $U = 4$ and 6 the development of sharp peaks is apparent. For $U = 4$ the peak-height converges to a non-zero value, implying a continuous transition at $V \approx 2.160$ with $K_\rho \approx 0.43$. For $U = 6$ the convergence to a value > 0 is not clear, but the transition point is given accurately by the peak-position, which shows very little size-dependence. It has been shown previously that the transition is first-order for $U = 6$ [6, 11], and the peak should therefore in fact converge to zero. The rather slow decay reflects the proximity to the point at which the transition becomes continuous. For $U = 8$ the peak does not sharpen, but instead a step develops at the critical V. The whole curve converges to 0 as $L \to \infty$. The

transition is hence strongly first-order in this case, in agreement with previous calculations. As seen in Fig. 1, and as observed already by Hirsch [6], the locations of the $U = 6$ and 8 critical points agree very well with the strong-coupling expansion [20].

In the SDW phase, one cannot expect to easily find $S_\sigma(q_1)/q_1 \to 1$ exactly, due to logarithmic corrections that affect various quantities strongly even for very long chains [21, 22]. However, the log-corrections are known to vanish in the frustrated $J - J'$ spin chain at its dimerization transition [23], and hence, since the SDW-BOW transition should be of the same nature, the log-corrections should vanish here as well. The transition at fixed U should therefore be signaled by $S_\sigma(q_1)/q_1$ crossing 1 from above as V is increased. Because of the vanishing log-corrections at the transition, the crossing point with 1 should not move significantly as L is increased, but the drop below 1 should become increasingly sharp, and eventually $S_\sigma(q_1)/q_1$ should approach 0 inside the BOW phase. This method was used in Ref. [11] and gave a slightly higher critical V for the SDW-BOW transition at $U = 4$ than the exact diagonalization [10]. We now have results for a wider range of couplings. The results shown in Fig. 2 are in accord with the above discussion for all three U-values; $S_\sigma(q_1)/q_1$ crosses 1 at a V-point which does not move visibly between $L = 64$ and $L = 256$. For larger V, one can see a sharper drop for the larger system sizes. The size dependence at $U = 4, V = 2.1$ is shown in an inset. Here the convergence to 0, i.e., the presence of a spin gap, is apparent. If the spin gap is small, as it is close to the phase boundary, the convergence to 0 will obviously occur only for very large systems.

Results such as those shown in Fig. 2 were used to determine the phase boundaries in Fig. 1. As already noted, the BOW aspect of the phase diagram differs from previous proposals [10, 11, 13, 14] in that the BOW-CDW transition can be either continuous or first-order, i.e., *the change of order occurs on the BOW-CDW boundary.* The existence of two special points, one where the transition-order changes and one at higher U where the BOW vanishes, was also suggested by Jeckelmann [14], who, however, insists that the BOW does not exist for small U where the transition to the CDW state is continuous (i.e., his phase diagram has no continuous BOW-CDW transition). We have carried out calculations for U down to 1, and, as shown in Fig. 1, we still find a BOW phase there. Most likely, in view also of weak-coupling arguments [13], the BOW extends down to $U = 0^+$. We find no BOW for $U \gtrsim 9$. In the strong-coupling expansion, using the couplings J and J' derived by van Dongen [8], the effective spin model is gapped, i.e., $J' > 0.241J$ [17], above the dashed curve in Fig. 1. The $J - J'$ mapping is not applicable beyond the transition into the CDW state, which (the solid curve in Fig. 1) was previously calculated by comparing the 4th-order CDW and $J - J'$ energies [8]. The 4th-order BOW region ends at $U \approx 7$, where the spin-gap curve crosses the CDW-transition curve. This is slightly lower than what we find based on QMC. The strong-coupling BOW extends down to smaller U, V, but clearly the 4th-order result cannot be expected to be quantitatively accurate in this region. Nevertheless, the spin-frustration mechanism consistently explains the presence of an SDW-BOW transition and an extended BOW phase. Spin-frustration was previously cited by Jeckelmann [14], but, surprisingly, he used it in support of a BOW of vanishing extent.

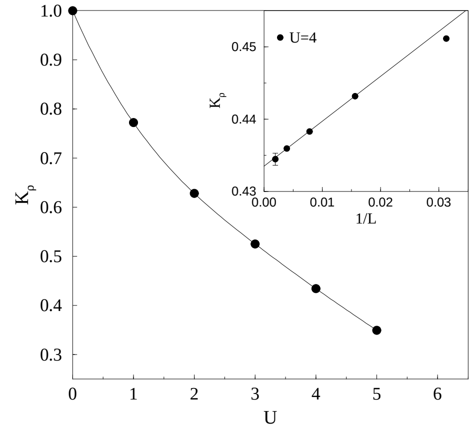

FIG. 3: QMC results for Luttinger charge exponent on the BOW-CDW boundary (solid circles). The inset shows the finite-size scaling for $U = 4$.

Next, we consider the nature of the BOW-CDW transition. As discussed in Refs. [10, 13], the continuous critical point for small U is described by a Gaussian free (charge) boson theory, characterized by the parameter K_ρ. At generic values of (repulsive) U, V, the leading "$4k_F$" umklapp process is present, and has scaling dimension $\Delta_{4k_F} = 2K_\rho$ and is hence relevant ($\Delta_{4k_F} < 2$) for $K_\rho < 1$. At the BOW-CDW transition, this operator vanishes, leading to a vanishing of the charge gap. For consistency, no other relevant operators should be present, which would otherwise require fine tuning to zero, making the Gaussian theory a multicritical point. The most dangerous candidate is the "$8k_F$" umklapp process, with $\Delta_{8k_F} = 4\Delta_{4k_F} = 8K_\rho$, so a continuous Gaussian critical point is possible only for $1 > K_\rho > 1/4$. Even in this range, the Gaussian theory is an unusual critical point with *non-universal* behavior, e.g., the correlation length exponent $\nu = 1/(2 - 2K_\rho)$.

Extrapolated QMC results for K_ρ on the BOW-CDW boundary are shown in Fig. 3. The finite-size corrections appear to be of the form $1/L^\alpha$, with an U dependent exponent α. At $U = 4$, $\alpha \approx 1$, as shown in the inset of Fig. 3. For larger U, α decreases rapidly and is difficult to determine accurately for $U \gtrsim 5$. The extrapolated K_ρ value at $U = 5$ in Fig. 3 should be regarded as an upper bound. At $U = 6$, the extrapolated $K_\rho < 1/4$, and hence we expect an eventual drop to 0. This is consistent

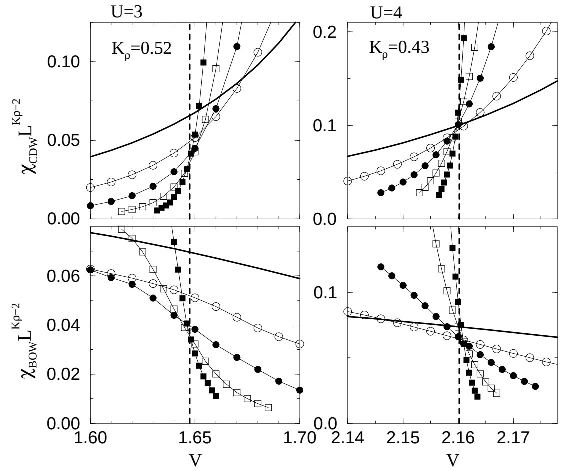

FIG. 4: Finite-size scaling of the BOW and CDW susceptibilities for $U = 3$ (left) and 4 (right). The symbols correspond to different system sizes as in Fig. 2. The dashed lines indicate the independently determined critical points.

with clear signals of a first-order transition [11]. Also at $U = 5.5$ there are signs of first-order behavior, e.g., in order parameter histograms such as those considered in Ref. 11. We believe that the change from a continuous to a first-order transition occurs between $U = 5$ and 5.5.

What is the nature of the tricritical point at which the transition becomes first-order? The simplest scenario is that this is the last (marginally) stable point of the Gaussian fixed line, i.e. with $K_\rho = 1/4$. This hypothesis predicts that the critical K_ρ continuously approaches 1/4 as the tricritical point $U = U_t$ is approached from below, as $K_\rho - 1/4 \sim \sqrt{(U_t - U)/U_t}$. We do not have sufficient data to verify this form, but it is consistent with a sharp drop to 0 between $U = 5$ and 5.5 (Fig. 3), required since at $U = 5.5$ the transition should be first-order. Hence, we favor this behavior over the a priori consistent (but less simple) possibility of a non-trivial "strong coupling" tricritical fixed point far from the Gaussian line.

To further demonstrate the Luther-Emery state on the continuous BOW-CDW curve, we study the finite-size scaling of the CDW and BOW susceptibilities, $\chi_{\rm CDW}(\pi)$ and $\chi_{\rm BOW}(\pi)$ (with their standard Kubo-integral definitions [11]). Both the charge and bond correlations should decay as $(-1)^r r^{-K_\rho}$ [18], implying that the susceptibilities scale with system size as L^{2-K_ρ}. Thus, $\chi(\pi)L^{K_\rho-2}$ curves for different L should intersect at the critical BOW-CDW point. Fig. 4 shows results for $U = 3$ and 4, using the K_ρ values determined above. For $U = 4$ the expected scaling can be observed even for small systems. For $U = 3$ the corrections are larger, and the asymptotic scaling sets in only for $L \gtrsim 128$. This is clearly due to the smaller spin gap at $U = 3$, which implies a longer length-scale below which remaining spin correlations affect the charge and bond fluctuations.

In summary, we have determined the ground state phase diagram of the extended Hubbard model at half-filling. The dimerized BOW phase can be explained by spin-frustration. The BOW-CDW transition changes from continuous to first-order between $U = 5$ and 5.5. On the critical (U, V) curve the system is a Luther-Emery liquid, with a charge exponent K_ρ decreasing from 1 as U is increased from 0. We have argued that the minimum $K_\rho = 1/4$ and that the BOW-CDW transition becomes first-order when this value is reached.

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